

=> d his

(FILE 'HOME' ENTERED AT 08:28:57 ON 15 JUN 2007)

FILE 'REGISTRY' ENTERED AT 08:29:10 ON 15 JUN 2007

L1 STRUCTURE UPLOADED
L2 0 S L1 SSS SAM
L3 3 S L1 SSS FULL

FILE 'CAPLUS' ENTERED AT 08:31:07 ON 15 JUN 2007

L4 4 S L3

FILE 'REGISTRY' ENTERED AT 08:33:14 ON 15 JUN 2007

L5 1 S 61581-05-3/RN

FILE 'CAPLUS' ENTERED AT 08:33:56 ON 15 JUN 2007

L6 0 S L5 AND "TRANSITION TEMPERATURE"
L7 140091 S "TRANSITION TEMPERATURE"
L8 101545 S HYDRATE
L9 0 S L5 AND L8
L10 228517 S ANHYDRIDE
L11 2184 S L8 AND L10
L12 0 S L11 AND L5
L13 0 S L5 AND PRECIPITATION
L14 0 S L5 AND PRECIPITATING
L15 0 S L5/RGT
L16 0 S L5/PREP
L17 0 S L5/PROC
L18 0 S L5/PUR
L19 0 S L5 AND PARAHYDROXYBENZOIC

FILE 'CASREACT' ENTERED AT 08:47:29 ON 15 JUN 2007

L20 0 S L5
E L5
L21 193 S E3 OR E6

FILE 'CAPLUS' ENTERED AT 08:49:45 ON 15 JUN 2007

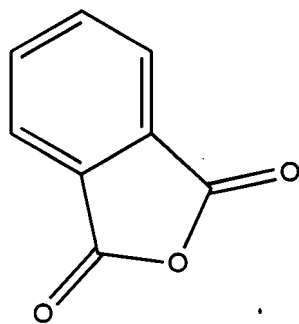
L22 193 S L21
L23 1 S L22 AND L7
L24 0 S L22 AND PRECIPITATING
L25 1 S L7 AND L22

FILE 'STNGUIDE' ENTERED AT 08:51:44 ON 15 JUN 2007

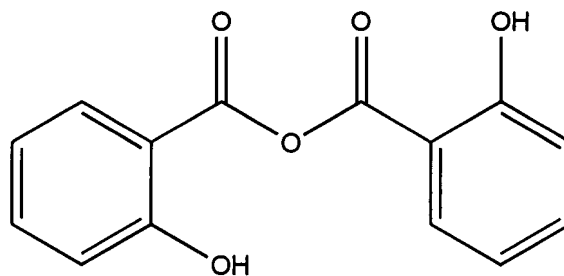
STN Search (add'l)

6/15/07

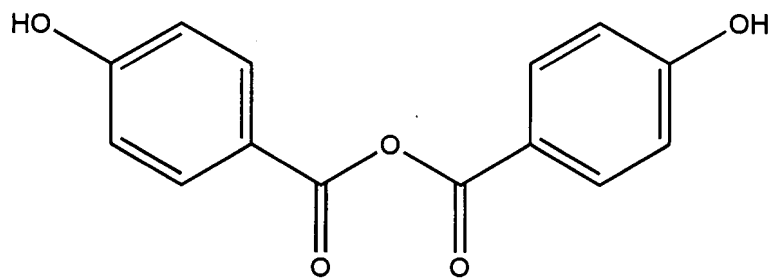
mu



phthalic anhydride

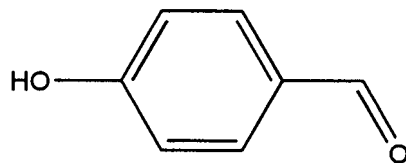


hydroxybenzoic anhydride



para-hydroxybenzoic anhydride

SN 10/553451



para-hydroxybenzoic acid monohydride

=> e US20060264670/apps

E1	1	US2006-DS248308/PRN
E2	1	US2006-DS259834/PRN
E3	0 -->	US20060264670/AP
E4	0	US20060264670/PRN
E5	1	US2007-528724/AP
E6	1	US2007-530406/AP
E7	1	US2007-530492/AP
E8	1	US2007-531465/AP
E9	1	US2007-532703/AP
E10	1	US2007-539995/AP
E11	1	US2007-541273/AP
E12	1	US2007-542249/AP

=> e US2006-264670/apps

E1	1	US2006-251648/AP
E2	1	US2006-256007/AP
E3	0 -->	US2006-264670/AP
E4	0	US2006-264670/PRN
E5	1	US2006-264673/AP
E6	1	US2006-265883/AP
E7	1	US2006-271355/AP
E8	1	US2006-274942/AP
E9	1	US2006-275437/AP
E10	1	US2006-275438/AP
E11	1	US2006-275439/AP
E12	1	US2006-275453/AP

=> s US2006-264670/apps

	0	US2006-264670/AP
	0	US2006-264670/PRN
L26	0	US2006-264670/APPS
		(US2006-264670/AP,PRN)

=> e US20060264670/apn,prn,pn

'APN' IS NOT A VALID EXPAND FIELD CODE FOR FILE 'CAPLUS'

E1	1	US2006026035/PN
E2	1	US2006026040/PN
E3	0 -->	US20060264670/PRN
E4	0	US20060264670/PN
E5	1	US2006026610/PN
E6	1	US2006026622/PN
E7	1	US2006026694/PN
E8	1	US2006026695/PN
E9	1	US2006026696/PN
E10	1	US2006026697/PN
E11	1	US2006026699/PN
E12	1	US2006026700/PN

The indicated field code is not available for EXPAND in this file. To see a list of valid EXPAND field codes, enter HELP SFIELDS at an arrow prompt (=>).

10/553451 CRYs p-HYDROXYBENZOIC ACID ANHYDRIDE - structure

=>

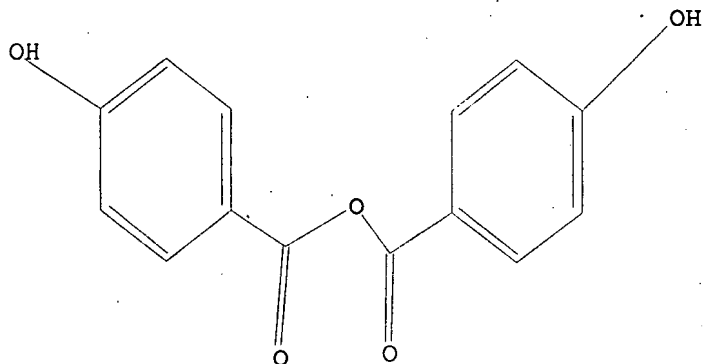
Uploading C:\Program Files\Stnexp\Queries\2007 cases\10553451\parahydroxybenzoic anhydride.str

L1 STRUCTURE UPLOADED

=> d l1

L1 HAS NO ANSWERS

L1 STR



Structure attributes must be viewed using STN Express query preparation.

=> s l1 sss sam

SAMPLE SEARCH INITIATED 08:29:33 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 849 TO ITERATE

100.0% PROCESSED 849 ITERATIONS

0 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**

PROJECTED ITERATIONS: 15232 TO 18728

PROJECTED ANSWERS: 0 TO 0

L2 0 SEA SSS SAM L1

=> s l1 sss full

FULL SEARCH INITIATED 08:29:42 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 17618 TO ITERATE

100.0% PROCESSED 17618 ITERATIONS

3 ANSWERS

SEARCH TIME: 00.00.01

L3 3 SEA SSS FUL L1

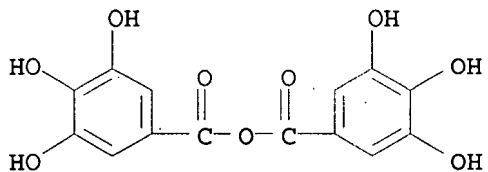
=> d scan

L3 3 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN

IN Benzoic acid, 3,4,5-trihydroxy-, anhydride (9CI)

MF C14 H10 O9

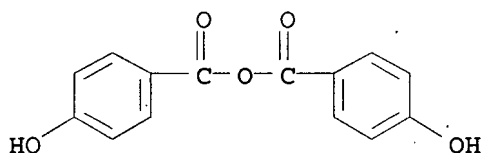
10/553451 CRYSTAL p-HYDROXYBENZOIC ACID ANHYDRIDE - structure



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):3

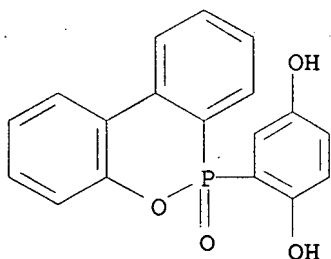
L3 3 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN
IN Benzoic acid, 4-hydroxy-, anhydride (9CI)
MF C14 H10 O5
CI COM



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

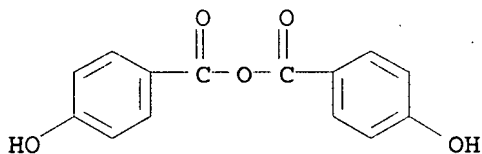
L3 3 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN
IN 1,4-Benzenedicarboxylic acid, polymer with 4-hydroxybenzoic acid anhydride
and 2-(6-oxido-6H-dibenz[c,e][1,2]oxaphosphorin-6-yl)-1,4-benzenediol
(9CI)
MF (C18 H13 O4 P . C14 H10 O5 . C8 H6 O4)x
CI PMS

CM 1

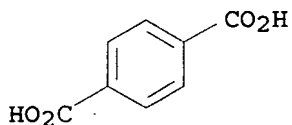


CM 2

10/553451 CRYs p-HYDROXYBENZOIC ACID ANHYDRIDE - structure



CM 3



ALL ANSWERS HAVE BEEN SCANNED

=> fil caplus
COST IN U.S. DOLLARS

SINCE FILE	TOTAL
ENTRY	SESSION
173.00	173.21

FULL ESTIMATED COST

FILE 'CAPLUS' ENTERED AT 08:31:07 ON 15 JUN 2007
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FILE COVERS 1907 - 15 Jun 2007 VOL 146 ISS 25
FILE LAST UPDATED: 13 Jun 2007 (20070613/ED)

Effective October 17, 2005, revised CAS Information Use Policies apply. They are available for your review at:

<http://www.cas.org/infopolicy.html>

=> d his

(FILE 'HOME' ENTERED AT 08:28:57 ON 15 JUN 2007)

FILE 'REGISTRY' ENTERED AT 08:29:10 ON 15 JUN 2007

L1	STRUCTURE UPLOADED
L2	0 S L1 SSS SAM
L3	3 S L1 SSS FULL

FILE 'CAPLUS' ENTERED AT 08:31:07 ON 15 JUN 2007

=> s 13

L4 4 L3

=> d ibib abs 14 1-4 hitstr

L4 ANSWER 1 OF 4 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2004:328553 CAPLUS

DOCUMENT NUMBER: 141:64396

TITLE: A comparative study of quantitative structure-activity relationship methods based on gallic acid derivatives

AUTHOR(S): Huang, H.; Ou, W.; Zhao, J.; Chen, D.; Wang, L.

CORPORATE SOURCE: State Key Lab. Pollution Control and Resources Reuse, Sch. Environ., Nanjing Univ., Nanjing, Peop. Rep. China

SOURCE: SAR and QSAR in Environmental Research (2004), 15(2), 83-99

CODEN: SQERED; ISSN: 1062-936X

PUBLISHER: Taylor & Francis Ltd.

DOCUMENT TYPE: Journal

LANGUAGE: English

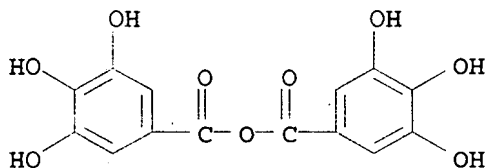
AB By using hologram quant. structure-activity relationship (HQSAR) and comparative mol. field anal. (CoMFA) methods, the relationships between the structures of 49 gallic acid derivs. and their analgesic activity have been investigated to yield statistically reliable models with considerable predictive power. The best HQSAR model was generated using atoms, bond and connectivity as fragment distinction parameters and fragment size 5-7 from a hologram length of 307 with 3 components. High conventional r^2 ($r^2=0.825$) and cross-validation r^2 ($rcv^2=0.726$) values were obtained. CoMFA analyses varying lattice size and location, grid spacing, probe charges and using, Tripos standard and Indicator force field were performed. The best model was developed with 4 components using sp^3 -hybridized carbon atom with +1.0 charge as probe, grid spacing (2 Å), lattice offset (1.0, 3.0, -2.5). The CoMFA model showed a conventional correlation coefficient r^2 of 0.889 and a cross-validation rcv^2 equals to 0.633. The robustness and predictive ability of the HQSAR and CoMFA models have been validated by means of an external test set. The results indicate that both models possess high statistical quality in the prediction of analgesic potency of novel gallic acid analogs.

IT 330664-37-4

RL: PAC (Pharmacological activity); BIOL (Biological study)
(comparative study of quant. structure-activity relationship methods based on gallic acid derivs.)

RN 330664-37-4 CAPLUS

CN Benzoic acid, 3,4,5-trihydroxy-, anhydride (9CI) (CA INDEX NAME)



REFERENCE COUNT: 23 THERE ARE 23 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 2 OF 4 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2001:26712 CAPLUS

DOCUMENT NUMBER: 134:231506

TITLE: Structure-activity relationships for the analgesic activity of gallic acid derivatives

AUTHOR(S): Krogh, R.; Yunes, R. A.; Andricopulo, A. D.

CORPORATE SOURCE: College of Pharmacy, University of Michigan, Ann Arbor, MI, 48109, USA

SOURCE: Farmaco (2000), 55(11-12), 730-735
CODEN: FRMCE8; ISSN: 0014-827X

PUBLISHER: Elsevier Science S.A.

DOCUMENT TYPE: Journal

LANGUAGE: English

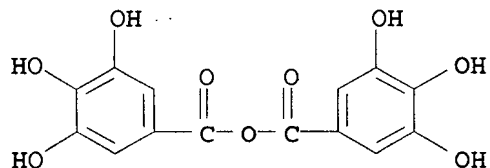
AB Values of ID50 for a collection of structurally-related gallic acid derivs. have been employed to create a predictive quant. structure-activity relation (QSAR) which links structure to values of analgesic activity. The QSAR model developed has substantial predictive power for the design of novel gallic acid derivs. having improved analgesic potency.

IT 330664-37-4

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PRP (Properties); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(structure-activity relationships for analgesic activity of gallic acid derivs.)

RN 330664-37-4 CAPLUS

CN Benzoic acid, 3,4,5-trihydroxy-, anhydride (9CI) (CA INDEX NAME)



REFERENCE COUNT: 11 THERE ARE 11 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 3 OF 4 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1987:619080 CAPLUS

DOCUMENT NUMBER: 107:219080

TITLE: Manufacture of aromatic polyester fibers

INVENTOR(S): Matsumoto, Tetsuo; Makita, Hirotoshi; Kagawa, Yoshifumi

PATENT ASSIGNEE(S): Japan Ester Co., Ltd., Japan

SOURCE: Jpn. Kokai Tokkyo Koho, 7 pp.

CODEN: JKXXAF

DOCUMENT TYPE: Patent

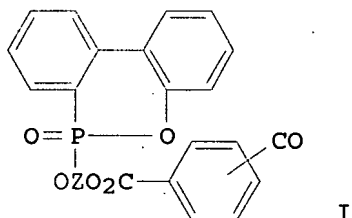
LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 62177211	A	19870804	JP 1986-17501	19860129
PRIORITY APPLN. INFO.:			JP 1986-17501	19860129

GI



AB High-tenacity aromatic polyester fibers are prepared by melt spinning thermotropic liquid-crystal-formable aromatic polyesters containing 5-95 mol% I units (Z = trivalent aromatic group) at draft ratio ≥ 5 , passing the fibers through gas heated above the softening temperature (Is) of the polyester,

and finally passing them through gas heated above the glass transition temperature (Ig) of the polyester. Thus, a 2.5:7.5:2 (mole ratio) mixture of 9,10-dihydro-9-oxa-10-(2',5'-dihydroxyphenyl)phosphaphenanthrene 10-oxide (II), 4-hydroxybenzoic anhydride, and acetic anhydride and 1 mol/mol II terephthalic acid were copolymerized to give an aromatic polyester (III). III (Ts 265°; Tg 186°) was spun at 330° and draft ratio 25, passed through gas at 275°, and subsequently passed through gas at 200° to give fibers with tenacity 14.7 g/denier and modulus 268 g/denier, vs. 2.8 g/denier and 205 g/denier, resp., for fibers spun at draft ratio 3.

IT 111523-01-4

RL: USES (Uses)

(fiber, melt spinning of, with high tenacity and modulus, draw ratio and heat-treatment temps. in relation to)

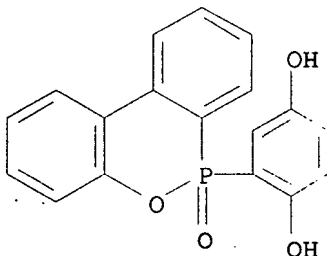
RN 111523-01-4 CAPLUS

CN 1,4-Benzenedicarboxylic acid, polymer with 4-hydroxybenzoic acid anhydride and 2-(6-oxido-6H-dibenz[c,e][1,2]oxaphosphorin-6-yl)-1,4-benzenediol (9CI) (CA INDEX NAME)

CM 1

CRN 99208-50-1

CMF C18 H13 O4 P

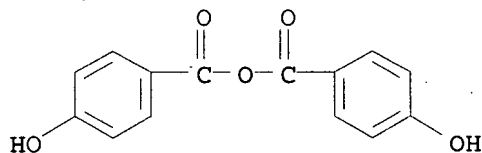


CM 2

CRN 61581-05-3

10/553451 CRYST p-HYDROXYBENZOIC ACID ANHYDRIDE - structure

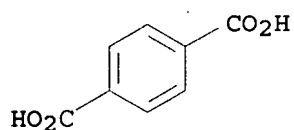
CMF C14 H10 O5



CM 3

CRN 100-21-0

CMF C8 H6 O4



L4 ANSWER 4 OF 4 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1977:55385 CAPLUS

DOCUMENT NUMBER: 86:55385

TITLE: Synthesis of compounds related to antitumor agents.
IV. On the reaction of aromatic carboxylates with
2,4-diamino-5-hydroxy-6-methylpyrimidine

AUTHOR(S): Kato, Tetsuo; Oda, Noriichi; Ito, Isao

CORPORATE SOURCE: Fac. Pharm. Sci., Nagoya City Univ., Nagoya, Japan

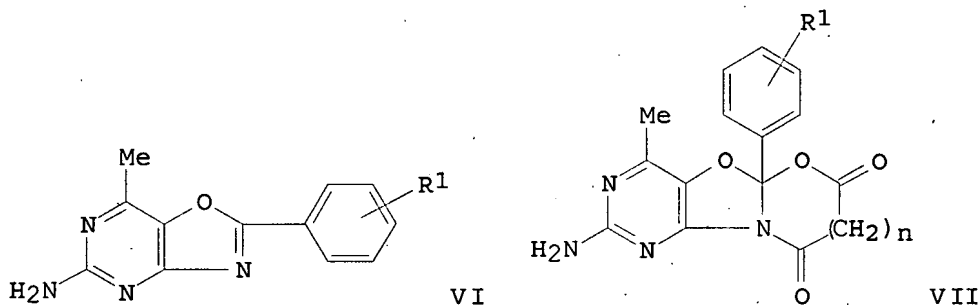
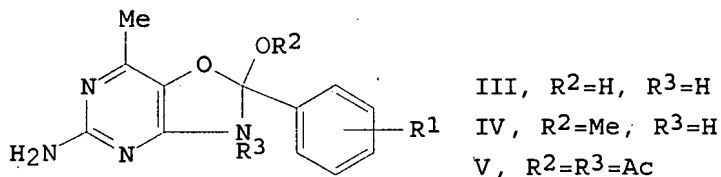
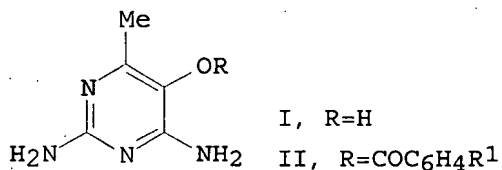
SOURCE: Chemical & Pharmaceutical Bulletin (1976), 24(10),
2461-9

CODEN: CPBTAL; ISSN: 0009-2363

DOCUMENT TYPE: Journal

LANGUAGE: English

GI



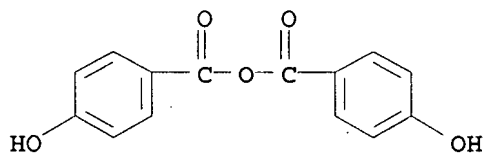
AB Reaction of the pyrimidine I with (R¹C₆H₄CO)₂O (R¹ = H, OH-o, -p, Me-o, -m, -p, NO₂-o, Cl-o) gave the corresponding II and the oxazolopyrimidines III. III were methylated (MeI), acetylated, dehydrated, or cyclized with ClCO(CH₂)_nCOCl (n = 1,2) to give IV-VII, resp.

IT 61581-05-3

RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction with diaminopyrimidinol)

RN 61581-05-3 CAPLUS

CN Benzoic acid, 4-hydroxy-, anhydride (9CI) (CA INDEX NAME)



=> fil reg

COST IN U.S. DOLLARS

FULL ESTIMATED COST

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

CA SUBSCRIBER PRICE

SINCE FILE

ENTRY

22.96

SINCE FILE

ENTRY

-3.12

TOTAL

SESSION

196.17

TOTAL

SESSION

-3.12

FILE 'REGISTRY' ENTERED AT 08:33:14 ON 15 JUN 2007

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10/553451 CRYSTAL p-HYDROXYBENZOIC ACID ANHYDRIDE - structure

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Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 14 JUN 2007 HIGHEST RN 937362-79-3

DICTIONARY FILE UPDATES: 14 JUN 2007 HIGHEST RN 937362-79-3

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TSCA INFORMATION NOW CURRENT THROUGH December 2, 2006

Please note that search-term pricing does apply when conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

<http://www.cas.org/support/stngen/stndoc/properties.html>

=> s 61581-05-3/rn

L5 1 61581-05-3/RN

=> d 15

L5 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2007 ACS on STN

RN 61581-05-3 REGISTRY

ED Entered STN: 16 Nov 1984

CN Benzoic acid, 4-hydroxy-, anhydride (9CI) (CA INDEX NAME)

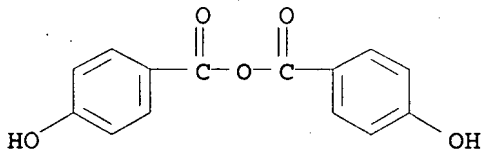
OTHER NAMES:

CN p-Hydroxybenzoic acid anhydride

MF C14 H10 O5

CI COM

LC STN Files: CA, CAPLUS, TOXCENTER



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

=> file caplu

COST IN U.S. DOLLARS

SINCE FILE	TOTAL
ENTRY	SESSION

FULL ESTIMATED COST

2.40	198.57
------	--------

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE	TOTAL
------------	-------

10/553451 CRYs p-HYDROXYBENZOIC ACID ANHYDRIDE - structure

	ENTRY	SESSION
CA SUBSCRIBER PRICE	0.00	-3.12

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FILE COVERS 1907 - 15 Jun 2007 VOL 146 ISS 25
FILE LAST UPDATED: 13 Jun 2007 (20070613/ED)

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=> d his

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L1 STRUCTURE UPLOADED
L2 0 S L1 SSS SAM
L3 3 S L1 SSS FULL

FILE 'CAPLUS' ENTERED AT 08:31:07 ON 15 JUN 2007

L4 4 S L3

FILE 'REGISTRY' ENTERED AT 08:33:14 ON 15 JUN 2007

L5 1 S 61581-05-3/RN

FILE 'CAPLUS' ENTERED AT 08:33:56 ON 15 JUN 2007

=> s l5 and "transition temperature"

1 L5
988581 "TRANSITION"
264538 "TRANSITIONS"
1102834 "TRANSITION"
("TRANSITION" OR "TRANSITIONS")
628632 "TEMPERATURE"
81658 "TEMPERATURES"
697936 "TEMPERATURE"
("TEMPERATURE" OR "TEMPERATURES")
3068948 "TEMP"
779803 "TEMPS"
3408904 "TEMP"
("TEMP" OR "TEMPS")
3568308 "TEMPERATURE"

10/553451 CRYs p-HYDROXYBENZOIC ACID ANHYDRIDE - structure

```
      ("TEMPERATURE" OR "TEMP")
140091 "TRANSITION TEMPERATURE"
      ("TRANSITION"(W) "TEMPERATURE")
L6      0 L5 AND "TRANSITION TEMPERATURE"

=> s "transition temperature"
      988581 "TRANSITION"
      264538 "TRANSITIONS"
      1102834 "TRANSITION"
            ("TRANSITION" OR "TRANSITIONS")
      628632 "TEMPERATURE"
      81658 "TEMPERATURES"
      697936 "TEMPERATURE"
            ("TEMPERATURE" OR "TEMPERATURES")
      3068948 "TEMP"
      779803 "TEMPS"
      3408904 "TEMP"
            ("TEMP" OR "TEMPS")
      3568308 "TEMPERATURE"
            ("TEMPERATURE" OR "TEMP")
L7      140091 "TRANSITION TEMPERATURE"
            ("TRANSITION"(W) "TEMPERATURE")
```

```
=> s hydrate
      86394 HYDRATE
      28916 HYDRATES
L8      101545 HYDRATE
            (HYDRATE OR HYDRATES)
```

```
=> s l5 and l8
      1 L5
L9      0 L5 AND L8
```

```
=> s anhydride
      217738 ANHYDRIDE
      33390 ANHYDRIDES
L10      228517 ANHYDRIDE
            (ANHYDRIDE OR ANHYDRIDES)
```

=> d his

(FILE 'HOME' ENTERED AT 08:28:57 ON 15 JUN 2007)

FILE 'REGISTRY' ENTERED AT 08:29:10 ON 15 JUN 2007

```
L1      STRUCTURE UPLOADED
L2      0 S L1 SSS SAM
L3      3 S L1 SSS FULL
```

FILE 'CAPLUS' ENTERED AT 08:31:07 ON 15 JUN 2007

```
L4      4 S L3
```

FILE 'REGISTRY' ENTERED AT 08:33:14 ON 15 JUN 2007

```
L5      1 S 61581-05-3/RN
```

FILE 'CAPLUS' ENTERED AT 08:33:56 ON 15 JUN 2007

```
L6      0 S L5 AND "TRANSITION TEMPERATURE"
L7      140091 S "TRANSITION TEMPERATURE"
L8      101545 S HYDRATE
L9      0 S L5 AND L8
```

10/553451 CRYs p-HYDROXYBENZOIC ACID ANHYDRIDE - structure

L10 228517 S ANHYDRIDE

=> s l8 and l10

L11 2184 L8 AND L10

=> s l11 and l5

1 L5

L12 0 L11 AND L5

=> help operators

The following operators are available for use in searching: 'AND', 'OR', 'NOT', (W), (NOTW), (A), (NOTA), (P), (NOTP), (S), (NOTS), (L), (NOTL) and numeric operators. The order of precedence for the execution of operators is (highest first): numeric operators; (W), (NOTW), (A), and (NOTA); (S) and (NOTS); (P) and (NOTP); (L) and (NOTL); 'AND' and 'NOT'; then 'OR'. Parentheses (nesting) can be used to alter the order of execution. For example, the expression

=> SEARCH A AND B OR C NOT D

is equivalent to

=> SEARCH (A AND B) OR (C NOT D).

If the search logic required the set 'B OR C' to be combined with set A by 'AND' logic and set D by 'NOT' logic, parentheses would be required as shown below to produce the desired results.

=> SEARCH A AND (B OR C) NOT D

For more information on the individual operators, enter "HELP" and one of the following at an arrow prompt (=>): 'NUMERIC', '(NOTPROXIMITY)', 'AND', 'OR', 'NOT', '(W)', '(A)', '(S)', '(P)', or '(L)'. Information on specific negative proximity operators is found with the corresponding positive proximity operator; e.g., for information on (NOTW), enter "HELP (W)". The numeric, Boolean, and (A), (NOTA), (W), and (NOTW) word proximity operators work the same in all files. However, the function of the (S), (NOTS), (P), (NOTP), (L), and (NOTL) operators depends on the data structure of the file you are in. Entering "HELP (S)", "HELP (P)", or "HELP (L)" will give information about how these operators work in the current file.

=> d his

(FILE 'HOME' ENTERED AT 08:28:57 ON 15 JUN 2007)

FILE 'REGISTRY' ENTERED AT 08:29:10 ON 15 JUN 2007

L1 STRUCTURE UPLOADED

L2 0 S L1 SSS SAM

L3 3 S L1 SSS FULL

FILE 'CAPLUS' ENTERED AT 08:31:07 ON 15 JUN 2007

L4 4 S L3

FILE 'REGISTRY' ENTERED AT 08:33:14 ON 15 JUN 2007

L5 1 S 61581-05-3/RN

FILE 'CAPLUS' ENTERED AT 08:33:56 ON 15 JUN 2007

L6 0 S L5 AND "TRANSITION TEMPERATURE"

10/553451 CRYs p-HYDROXYBENZOIC ACID ANHYDRIDE - structure

L7 140091 S "TRANSITION TEMPERATURE"
L8 101545 S HYDRATE
L9 0 S L5 AND L8
L10 228517 S ANHYDRIDE
L11 2184 S L8 AND L10
L12 0 S L11 AND L5

=> s l5 and precipitation

1 L5
68195 PRECIPITATION
664 PRECIPITATIONS
68699 PRECIPITATION
(PRECIPITATION OR PRECIPITATIONS)
267038 PPTN
4375 PPTNS
269755 PPTN
(PPTN OR PPTNS)
291316 PRECIPITATION
(PRECIPITATION OR PPTN)
L13 0 L5 AND PRECIPITATION

=> s l5 and precipitating

1 L5
4403 PRECIPITATING
38040 PPTG
41350 PRECIPITATING
(PRECIPITATING OR PPTG)
L14 0 L5 AND PRECIPITATING

=> s l5/rgt

1 L5
46138 RGT/RL
L15 0 L5/RGT
(L5 (L) RGT/RL)

=> s l5/prep

1 L5
4417183 PREP/RL
L16 0 L5/PREP
(L5 (L) PREP/RL)

=> s l5/proc

1 L5
4118363 PROC/RL
L17 0 L5/PROC
(L5 (L) PROC/RL)

=> s l5/pur

1 L5
257574 PUR/RL
L18 0 L5/PUR
(L5 (L) PUR/RL)

=> s l5 and parahydroxybenzoic

1 L5
61 PARAHYDROXYBENZOIC
L19 0 L5 AND PARAHYDROXYBENZOIC

=> fil casreact

10/553451 CRYs p-HYDROXYBENZOIC ACID ANHYDRIDE - structure

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	36.94	235.51
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	0.00	-3.12

FILE 'CASREACT' ENTERED AT 08:47:29 ON 15 JUN 2007
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FILE CONTENT:1840 - 9 Jun 2007 VOL 146 ISS 25

New CAS Information Use Policies, enter HELP USAGETERMS for details.

```
*****
*
*   CASREACT now has more than 12 million reactions
*
*****
```

Some CASREACT records are derived from the ZIC/VINITI database (1974-1999) provided by InfoChem, INPI data prior to 1986, and Biotransformations database compiled under the direction of Professor Dr. Klaus Kieslich.

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> d his

(FILE 'HOME' ENTERED AT 08:28:57 ON 15 JUN 2007)

FILE 'REGISTRY' ENTERED AT 08:29:10 ON 15 JUN 2007

```
L1      STRUCTURE UPLOADED
L2      0 S L1 SSS SAM
L3      3 S L1 SSS FULL
```

FILE 'CAPLUS' ENTERED AT 08:31:07 ON 15 JUN 2007

```
L4      4 S L3
```

FILE 'REGISTRY' ENTERED AT 08:33:14 ON 15 JUN 2007

```
L5      1 S 61581-05-3/RN
```

FILE 'CAPLUS' ENTERED AT 08:33:56 ON 15 JUN 2007

```
L6      0 S L5 AND "TRANSITION TEMPERATURE"
L7      140091 S "TRANSITION TEMPERATURE"
L8      101545 S HYDRATE
L9      0 S L5 AND L8
L10     228517 S ANHYDRIDE
L11     2184 S L8 AND L10
L12     0 S L11 AND L5
L13     0 S L5 AND PRECIPITATION
L14     0 S L5 AND PRECIPITATING
```

10/553451 CRYSTAL p-HYDROXYBENZOIC ACID ANHYDRIDE - structure

L15 0 S L5/RGT
L16 0 S L5/PREP
L17 0 S L5/PROC
L18 0 S L5/PUR
L19 0 S L5 AND PARAHYDROXYBENZOIC

FILE 'CASREACT' ENTERED AT 08:47:29 ON 15 JUN 2007

=> s 15

L20 0 L5

=> e 15

E1 1 L4ZN8/BI
E2 1 L4ZNX2/BI
E3 166 --> L5/BI
E4 1 L50/BI
E5 1 L51784/BI
E6 27 L5178Y/BI
E7 1 L52/BI
E8 1 L5222/BI
E9 1 L52CU/BI
E10 1 L54MN4/BI
E11 1 L55/BI
E12 1 L56/BI

=> s e3 or e6

166 "L5"/BI
27 L5178Y/BI

L21 193 "L5"/BI OR L5178Y/BI

=> d scan

L21 193 ANSWERS CASREACT COPYRIGHT 2007 ACS on STN

TI Extraction and coordination studies of the unexplored bifunctional ligand carbamoyl methyl sulfoxide (CMSO) with uranium(VI) and cerium(III) nitrates. Synthesis and structures of $[\text{UO}_2(\text{NO}_3)_2(\text{PhSOCH}_2\text{CONiBu}_2)]$ and $[\text{Ce}(\text{NO}_3)_3(\text{PhSOCH}_2\text{CONBu}_2)_2]$
NO HIGHLIGHTING INFORMATION PRESENT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):5

L21 193 ANSWERS CASREACT COPYRIGHT 2007 ACS on STN

TI Synthesis, coordination to Rh(I), and hydroformylation catalysis of new β -aminophosphines bearing a dangling nitrogen group: an unusual inversion of a Rh-coordinated P center
NO HIGHLIGHTING INFORMATION PRESENT

L21 193 ANSWERS CASREACT COPYRIGHT 2007 ACS on STN

TI Sparsomycin analogs. V. Synthesis and antitumor activity of (E)- β -(pyrimidin-5-yl)acrylamides
NO HIGHLIGHTING INFORMATION PRESENT

L21 193 ANSWERS CASREACT COPYRIGHT 2007 ACS on STN

TI Betaine-induced assembly of neutral infinite columns and chains of linked silver(I) polyhedra with embedded acetylenediide

NO HIGHLIGHTING INFORMATION PRESENT

L21 193 ANSWERS CASREACT COPYRIGHT 2007 ACS on STN

TI Cobalt(II) and manganese(II) complexes of unsymmetric compartmental ligands bearing adjacent {N2O} and {N,S,O} donor sets
NO HIGHLIGHTING INFORMATION PRESENT

L21 193 ANSWERS CASREACT COPYRIGHT 2007 ACS on STN

TI Macrocyclic thioether-esters and thioether-thioesters and their palladium, platinum and silver complexes
NO HIGHLIGHTING INFORMATION PRESENT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):0

=> d l21 it

L21 ANSWER 1 OF 193 CASREACT COPYRIGHT 2007 ACS on STN

IT Michaelis constant
(kinetic parameters of protein kinases; preparation of nitrogen heterocyclic ruthenium metal complexes as glycogen synthase kinase 3 inhibitors)

IT Crystal structure
Molecular structure
(of pyridocarbazole cyclopentadienylruthenium complex)

IT Human
(preparation of nitrogen heterocyclic ruthenium metal complexes as glycogen synthase kinase 3 inhibitors)

IT 936112-70-8P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(crystal structure; preparation of nitrogen heterocyclic ruthenium metal complexes as glycogen synthase kinase 3 inhibitors)

IT 936112-68-4P
RL: PEP (Physical, engineering or chemical process); PRP (Properties); SPN (Synthetic preparation); PREP (Preparation); PROC (Process)
(mol. structure, HPLC chromatog. separation of isomers; preparation of nitrogen heterocyclic ruthenium metal complexes as glycogen synthase kinase 3 inhibitors)

IT 90698-26-3 114051-78-4, Lck kinase 137632-07-6, Erk1 kinase
141436-78-4, Protein kinase Cα 144697-17-6, c-Src kinase
148047-34-1, ZAP-70 kinase 154907-65-0 391208-93-8, Glycogen synthase kinase 3 443900-95-6, Glycogen synthase kinase 3β 553648-93-4, Glycogen synthase kinase 3α
RL: BCP (Biochemical process); BIOL (Biological study); PROC (Process)
(preparation of nitrogen heterocyclic ruthenium metal complexes as glycogen synthase kinase 3 inhibitors)

IT 936232-98-3P 936233-00-0P
RL: BSU (Biological study, unclassified); PAC (Pharmacological activity); PUR (Purification or recovery); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of nitrogen heterocyclic ruthenium metal complexes as glycogen synthase kinase 3 inhibitors)

IT 852658-41-4P 936112-65-1P 936112-66-2P 936112-69-5P
RL: BSU (Biological study, unclassified); PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

10/553451 CRYs p-HYDROXYBENZOIC ACID ANHYDRIDE - structure

(preparation of nitrogen heterocyclic ruthenium metal complexes as glycogen synthase kinase 3 inhibitors)

IT 3724-16-1, 3-Pyridineacetamide 80049-63-4 259752-98-2 936112-71-9

RL: RCT (Reactant); RACT (Reactant or reagent)

(preparation of nitrogen heterocyclic ruthenium metal complexes as glycogen synthase kinase 3 inhibitors)

IT 799822-53-0P 799822-54-1P 799822-55-2P 799822-56-3P 799822-57-4P

799822-58-5P 936112-67-3P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of nitrogen heterocyclic ruthenium metal complexes as glycogen synthase kinase 3 inhibitors)

=> d his

(FILE 'HOME' ENTERED AT 08:28:57 ON 15 JUN 2007)

FILE 'REGISTRY' ENTERED AT 08:29:10 ON 15 JUN 2007

L1 STRUCTURE UPLOADED

L2 0 S L1 SSS SAM

L3 3 S L1 SSS FULL

FILE 'CAPLUS' ENTERED AT 08:31:07 ON 15 JUN 2007

L4 4 S L3

FILE 'REGISTRY' ENTERED AT 08:33:14 ON 15 JUN 2007

L5 1 S 61581-05-3/RN

FILE 'CAPLUS' ENTERED AT 08:33:56 ON 15 JUN 2007

L6 0 S L5 AND "TRANSITION TEMPERATURE"

L7 140091 S "TRANSITION TEMPERATURE"

L8 101545 S HYDRATE

L9 0 S L5 AND L8

L10 228517 S ANHYDRIDE

L11 2184 S L8 AND L10

L12 0 S L11 AND L5

L13 0 S L5 AND PRECIPITATION

L14 0 S L5 AND PRECIPITATING

L15 0 S L5/RGT

L16 0 S L5/PREP

L17 0 S L5/PROC

L18 0 S L5/PUR

L19 0 S L5 AND PARAHYDROXYBENZOIC

FILE 'CASREACT' ENTERED AT 08:47:29 ON 15 JUN 2007

L20 0 S L5

E L5

L21 193 S E3 OR E6

=> fil caplus

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

35.02

270.53

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE

TOTAL

ENTRY

SESSION

CA SUBSCRIBER PRICE

0.00

-3.12

10/553451 CRYSTAL p-HYDROXYBENZOIC ACID ANHYDRIDE - structure

FILE 'CAPLUS' ENTERED AT 08:49:45 ON 15 JUN 2007

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FILE COVERS 1907 - 15 Jun 2007 VOL 146 ISS 25

FILE LAST UPDATED: 13 Jun 2007 (20070613/ED)

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<http://www.cas.org/infopolicy.html>

=> s 121

L22 193 L21

=> s 122 and 17

L23 1 L22 AND L7

=> d ibib abs

L23 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2005:1046581 CAPLUS

DOCUMENT NUMBER: 144:15951

TITLE: Lanthanide luminescent mesomorphic complexes with macrocycles derived from diaza-18-crown-6

AUTHOR(S): Suarez, Stephane; Mamula, Olimpia; Scopelliti, Rosario; Donnio, Bertrand; Guillon, Daniel; Terazzi, Emmanuel; Piguet, Claude; Buezli, Jean-Claude G.

CORPORATE SOURCE: Laboratory of Lanthanide Supramolecular Chemistry, BCH 1402, Ecole Polytechnique Federale de Lausanne (EPFL), Lausanne, CH-1015, Switz.

SOURCE: New Journal of Chemistry (2005), 29(10), 1323-1334

CODEN: NJCHE5; ISSN: 1144-0546

PUBLISHER: Royal Society of Chemistry

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 144:15951

GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Four tetracatenar (L1-L4; I, Z = CH₂, CO; R = OMe, OC10H₂₁, OC12H₂₅, OC18H₃₃) and one hexacatenar (L5; II) ligands, derived from the diaza-18-crown-6 framework, were synthesized and characterized. In these

ligands, the amine functions are fitted with benzoyloxybenzyl linker groups, attached either with a carbonyl function (L1) or a methylene bridge (L2-L5) and bearing alkoxy chains, R, of various lengths: R = OCH₃ for L2, OC10H₂₁ for L3 and L5, OC12H₂₅ for L1, and OC16H₃₃ for L4. The nonmesomorphic ligands L1 and L3-L5 react with various lanthanide salts to give complexes forming thermotropic hexagonal columnar phases, as ascertained by thermal, optical and small-angle x-ray diffraction methods. The length of the alkoxy chains (L3 and L4) does not much influence the mesogenic behavior, irrespectively of the linker function, the number of alkoxy chains, the counterion or the lanthanide ion. The best systems proved to be the nitrate lanthanide complexes with L3, which present a Colh phase over 100° (up to 147° for La) with melting transition temps. between 58 (La) and 86 (Tb) °C. In the case of [Eu(NO₃)₃L3], chosen as a representative example of all the complexes in this anal., the inter-column separation of 29.2 Å agrees well with the packing of cylindrical columns resulting from an alternated stacking of the mols., in which the two mesogenic arms extend on the same side, i.e. stacking the mols. in a bent conformation. The liquid crystalline phases containing Eu and Tb display metal-centered emission, meaning that these complexes are interesting building blocks for the design of luminescent liquid crystalline materials.

REFERENCE COUNT: 57 THERE ARE 57 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> s l22 and precipitating
 4403 PRECIPITATING
 38044 PPTG
 41354 PRECIPITATING
 (PRECIPITATING OR PPTG)
 L24 0 L22 AND PRECIPITATING

=> s l7 and l22
 L25 1 L7 AND L22

=> d ibib abs

L25 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 2005:1046581 CAPLUS
 DOCUMENT NUMBER: 144:15951
 TITLE: Lanthanide luminescent mesomorphic complexes with macrocycles derived from diaza-18-crown-6
 AUTHOR(S): Suarez, Stephane; Mamula, Olimpia; Scopelliti, Rosario; Donnio, Bertrand; Guillon, Daniel; Terazzi, Emmanuel; Piguet, Claude; Buezli, Jean-Claude G.
 CORPORATE SOURCE: Laboratory of Lanthanide Supramolecular Chemistry, BCH 1402, Ecole Polytechnique Federale de Lausanne (EPFL), Lausanne, CH-1015, Switz.
 SOURCE: New Journal of Chemistry (2005), 29(10), 1323-1334
 CODEN: NJCHE5; ISSN: 1144-0546
 PUBLISHER: Royal Society of Chemistry
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 144:15951
 GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Four tetracatenar (L1-L4; I, Z = CH₂, CO; R = OMe, OC10H₂₁, OC12H₂₅, OC18H₃₃) and one hexacatenar (L5; II) ligands, derived from the diaza-18-crown-6 framework, were synthesized and characterized. In these ligands, the amine functions are fitted with benzyloxybenzyl linker groups, attached either with a carbonyl function (L1) or a methylene bridge (L2-L5) and bearing alkoxy chains, R, of various lengths: R = OCH₃ for L2, OC10H₂₁ for L3 and L5, OC12H₂₅ for L1, and OC16H₃₃ for L4. The nonmesomorphic ligands L1 and L3-L5 react with various lanthanide salts to give complexes forming thermotropic hexagonal columnar phases, as ascertained by thermal, optical and small-angle x-ray diffraction methods. The length of the alkoxy chains (L3 and L4) does not much influence the mesogenic behavior, irrespectively of the linker function, the number of alkoxy chains, the counterion or the lanthanide ion. The best systems proved to be the nitrate lanthanide complexes with L3, which present a Colh phase over 100° (up to 147° for La) with melting transition temps. between 58 (La) and 86 (Tb) °C. In the case of [Eu(NO₃)₃L3], chosen as a representative example of all the complexes in this anal., the inter-column separation of 29.2 Å agrees well with the packing of cylindrical columns resulting from an alternated stacking of the mols., in which the two mesogenic arms extend on the same side, i.e. stacking the mols. in a bent conformation. The liquid crystalline phases containing Eu and Tb display metal-centered emission, meaning that these complexes are interesting building blocks for the design of luminescent liquid crystalline materials.

REFERENCE COUNT: 57 THERE ARE 57 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> fil stng

COST IN U.S. DOLLARS

SINCE FILE	TOTAL
ENTRY	SESSION
9.08	279.61

FULL ESTIMATED COST

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE	TOTAL
ENTRY	SESSION
-1.56	-4.68

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FILE CONTAINS CURRENT INFORMATION.

LAST RELOADED: Jun 8, 2007 (20070608/UP).

=> d his

(FILE 'HOME' ENTERED AT 08:28:57 ON 15 JUN 2007)

FILE 'REGISTRY' ENTERED AT 08:29:10 ON 15 JUN 2007

L1	STRUCTURE UPLOADED
L2	0 S L1 SSS SAM
L3	3 S L1 SSS FULL

FILE 'CAPLUS' ENTERED AT 08:31:07 ON 15 JUN 2007

L4	4 S L3
----	--------

FILE 'REGISTRY' ENTERED AT 08:33:14 ON 15 JUN 2007

10/553451 CRYs p-HYDROXYBENZOIC ACID ANHYDRIDE - structure

L5 1 S 61581-05-3/RN

FILE 'CAPLUS' ENTERED AT 08:33:56 ON 15 JUN 2007

L6 0 S L5 AND "TRANSITION TEMPERATURE"

L7 140091 S "TRANSITION TEMPERATURE"

L8 101545 S HYDRATE

L9 0 S L5 AND L8

L10 228517 S ANHYDRIDE

L11 2184 S L8 AND L10

L12 0 S L11 AND L5

L13 0 S L5 AND PRECIPITATION

L14 0 S L5 AND PRECIPITATING

L15 0 S L5/RGT

L16 0 S L5/PREP

L17 0 S L5/PROC

L18 0 S L5/PUR

L19 0 S L5 AND PARAHYDROXYBENZOIC

FILE 'CASREACT' ENTERED AT 08:47:29 ON 15 JUN 2007

L20 0 S L5

E L5

L21 193 S E3 OR E6

FILE 'CAPLUS' ENTERED AT 08:49:45 ON 15 JUN 2007

L22 193 S L21

L23 1 S L22 AND L7

L24 0 S L22 AND PRECIPITATING

L25 1 S L7 AND L22

FILE 'STNGUIDE' ENTERED AT 08:51:44 ON 15 JUN 2007

10/553451 Crys p-HYDROXYBENZOIC ACID ANHYDRIDE - structure

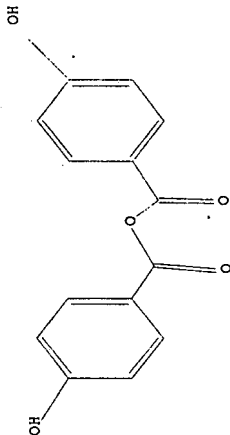
=> Uploading C:\Program Files\Stnexp\Queries\2007 cases\10553451\parahydroxybenzoic anhydride.str

L1 STRUCTURE UPLOADED

=> d l1

L1 HAS NO ANSWERS

L1 STR



Structure attributes must be viewed using STN Express query preparation.

=> s l1 sss sam
SAMPLE SEARCH INITIATED 08:29:33 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 849 TO ITERATE

0 ANSWERS

100.0% PROCESSED 849 ITERATIONS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

PROJECTED ITERATIONS: BATCH **COMPLETE**

PROJECTED ANSWERS: 15232 TO 18728
0 TO 0

L2 0 SEA SSS SAM L1

=> s l1 sss full

FULL SEARCH INITIATED 08:29:42 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 17618 TO ITERATE

3 ANSWERS

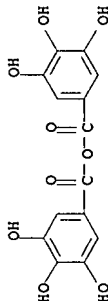
100.0% PROCESSED 17618 ITERATIONS
SEARCH TIME: 00.00.01

L3 3 SEA SSS FUL L1

=> d scan

L3 3 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN
IN Benzoic acid, 3,4,5-trihydroxy-, anhydride (9CI)
MF C14 H10 O9

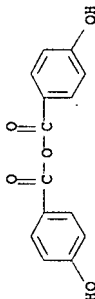
10/553451 Crys p-HYDROXYBENZOIC ACID ANHYDRIDE - structure



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):3

L3 3 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN
IN Benzoic acid, 4-hydroxy-, anhydride (9CI)
MF C14 H10 O5
CI COM



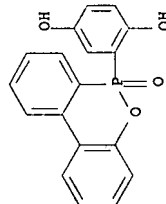
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 3 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN
IN 1,4-Benzenedicarboxylic acid, polymer with 4-hydroxybenzoic acid anhydride
and 2-(6-oxido-6H-dibenz[c,e][1,2]oxaphosphorin-6-yl)-1,4-benzenediol
(9CI)

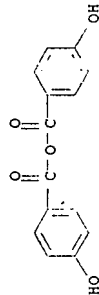
MF (C18 H13 O4 P . C14 H10 O5 . C8 H6 O4)x

CI PMS

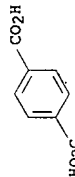
CM 1



CM 2



CM 3



ALL ANSWERS HAVE BEEN SCANNED

=> fil caplus
 COST IN U.S. DOLLARS
 FULL ESTIMATED COST
 SINCE FILE ENTRY
 173.00
 173.21
 TOTAL SESSION

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FILE COVERS 1907 - 15 Jun 2007 VOL 146 ISS 25
 FILE LAST UPDATED: 13 Jun 2007 (20070613/ED)

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<http://www.cas.org/infopolicy.html>

=> d his

(FILE 'HOME' ENTERED AT 08:28:57 ON 15 JUN 2007)

FILE 'REGISTRY' ENTERED AT 08:29:10 ON 15 JUN 2007
 L1 STRUCTURE UPLOADED
 L2 0 S L1 SSS SAM
 L3 3 S L1 SSS FULL

Page 3 searched 6/15/07

FILE 'CAPLUS' ENTERED AT 08:31:07 ON 15 JUN 2007

=> s L3
 L4 4 L3

=> d bib abs l4 l-4 hitstr

L4 ANSWER 1 OF 4 CAPLUS COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 2004:328553 CAPLUS
 DOCUMENT NUMBER: 141:64396

TITLE: A comparative study of quantitative structure-activity relationship methods based on gallic acid derivatives
 AUTHOR(S): Huang, H.; Ou, W.; Zhao, J.; Chen, D.; Wang, L.
 CORPORATE SOURCE: State Key Lab. Pollution Control and Resources Reuse, Sch. Environ., Nanjing Univ., Nanjing, Peop. Rep. China

SOURCE: SAR and QSAR in Environmental Research (2004), 15(2), 83-99
 CODEN: SQERED; ISSN: 1062-936X

PUBLISHER: Taylor & Francis Ltd.

DOCUMENT TYPE: Journal

LANGUAGE: English

AB By using hologram quant. structure-activity relationship (HQ SAR) and comparative mol. field anal. (CoMFA) methods, the relationships between the structures of 49 gallic acid derivs. and their analgesic activity have been investigated to yield statistically reliable models with considerable predictive power. The best HQ SAR model was generated using atoms, bond and connectivity as fragment distinction parameters and fragment size 5-7 from a hologram length of 307 with 3 components. High conventional r^2 ($r^2=0.825$) and cross-validation r^2 ($rcv^2=0.726$) values were obtained. CoMFA analyses varying lattice size and location, grid spacing, probe charges and using, Tripos standard and indicator force field were performed. The best model was developed with 4 components using sp³-hybridized carbon atom with +1.0 charge as probe, grid spacing (2 Å), lattice offset (1.0, 3.0, -2.5). The CoMFA model showed a conventional correlation coefficient r^2 of 0.889 and a cross-validation rcv^2 equals to 0.633. The robustness and predictive ability of the HQ SAR and CoMFA models have been validated by means of an external test set. The results indicate that both models possess high statistical quality in the prediction of analgesic potency of novel gallic acid analogs.

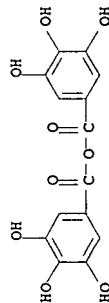
IT

RL: PAC (Pharmacological activity); BIOL (Biological study)

(comparative study of quant. structure-activity relationship methods based on gallic acid derivs.)

RN 330664-37-4 CAPLUS

CN Benzoic acid, 3,4,5-trihydroxy-, anhydride (9CI) (CA INDEX NAME)



REFERENCE COUNT:

23

THERE ARE 23 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

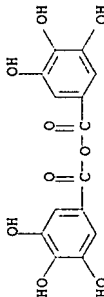
Page 4 searched 6/15/07

10/553451 CRY5 P-HYDROXYBENZOIC ACID ANHYDRIDE - structure

L4 ANSWER 2 OF 4 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2001:26712 CAPLUS
DOCUMENT NUMBER: 134:231506
TITLE: Structure-activity relationships for the analgesic activity of gallic acid derivatives
AUTHOR(S): Krogh, R.; Yunes, R. A.; Andricopulo, A. D.
CORPORATE SOURCE: College of Pharmacy, University of Michigan, Ann Arbor, MI, 48109, USA
SOURCE: Farmaco (2000), 55(11-12), 730-735
CODEN: FRMCE8; ISSN: 0014-827X
PUBLISHER: Elsevier Science S.A.
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Values of ID50 for a collection of structurally-related gallic acid derivs. have been employed to create a predictive quant. structure-activity relation (QSAR) which links structure to values of analgesic activity. The QSAR model developed has substantial predictive power for the design of novel gallic acid derivs. having improved analgesic potency.

IT 330664-37-4
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PRP (Properties); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(structure-activity relationships for analgesic activity of gallic acid derivs.)

RN 330664-37-4 CAPLUS
CN Benzoic acid, 3,4,5-trihydroxy-, anhydride (9CI) (CA INDEX NAME)



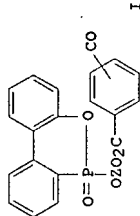
REFERENCE COUNT: 11 THERE ARE 11 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 3 OF 4 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1987:619080 CAPLUS
DOCUMENT NUMBER: 107:219080
TITLE: Manufacture of aromatic polyester fibers
INVENTOR(S): Matsumoto, Tetsuo; Makita, Hirotooshi; Kagawa, Yoshifumi
PATENT ASSIGNEE(S): Japan Ester Co., Ltd., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 7 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 62177211	A	19870804	JP 1986-17501	19860129
PRIORITY APPLN. INFO.:				19860129

10/553451 CRY5 P-HYDROXYBENZOIC ACID ANHYDRIDE - structure

GI

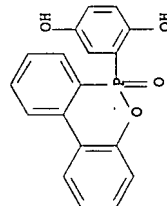


AB High-tenacity aromatic polyester fibers are prepared by melt spinning thermotropic liquid-crystal-formable aromatic polyesters containing 5-95 mol% I units (I = trivalent aromatic group) at draft ratio 25, passing the fibers through gas heated above the softening temperature (Is) of the polyester, and finally passing them through gas heated above the glass transition temperature (Ig) of the polyester. Thus, a 2.5:7.5:2 (mole ratio) mixture of 9,10-dihydro-9-oxa-10-[2',5'-dihydroxyphenyl]phosphanethrene 10-oxide (II), 4-hydroxybenzoic anhydride, and acetic anhydride and 1 mol/mol III terephthalic acid were copolymerized to give an aromatic polyester (III). III (Ts 265°; Tg 186°) was spun at 330° and draft ratio 25, passed through gas at 275°, and subsequently passed through gas at 200° to give fibers with tenacity 14.7 g/denier and modulus 268 g/denier, vs. 2.8 g/denier and 205 g/denier, resp., for fibers spun at draft ratio 3.

IT 111523-01-4
RL: USES (Uses)
(fiber, melt spinning of, with high tenacity and modulus, draw ratio and heat-treatment temps. in relation to)

RN 111523-01-4 CAPLUS
CN 1,4-Benzenedicarboxylic acid, polymer with 4-hydroxybenzoic acid anhydride and 2-(6-oxido-6H-dibenz[c,e][1,2]oxaphosphorin-6-yl)-1,4-benzenediol (9CI) (CA INDEX NAME)

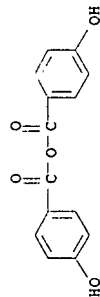
CM 1
CRN 99208-50-1
CMF C18 H13 O4 P



CM 2
CRN 61581-05-3

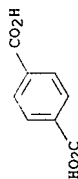
10/553451 Crys p-HYDROXYBENZOIC ACID ANHYDRIDE - structure

CMF C14 H10 O5



CM 3

CRN 100-21-0
CMF C8 H6 O4



L4 ANSWER 4 OF 4 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER:
DOCUMENT NUMBER:
TITLE:

1977:55385 CAPLUS

86:55385

Synthesis of compounds related to antitumor agents.
IV. On the reaction of aromatic carboxylates with
2,4-diamino-5-hydroxy-6-methylpyrimidine
Kato, Tetsuo; Oda, Noriichi; Ito, Isao
Fac. Pharm. Sci., Nagoya City Univ., Nagoya, Japan
Chemical & Pharmaceutical Bulletin (1976), 24(10),
2461-9

AUTHOR(S):
CORPORATE SOURCE:
SOURCE:

CODEN: CPBTAL; ISSN: 0009-2363

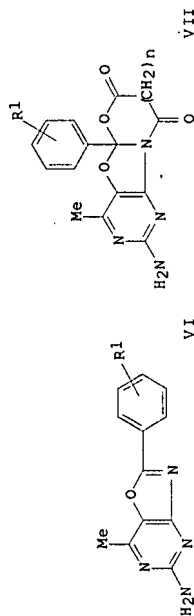
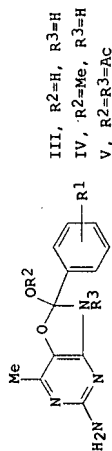
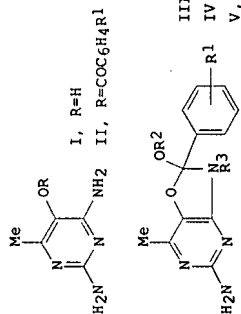
DOCUMENT TYPE:
LANGUAGE:

Journal

English

GI

10/553451 Crys p-HYDROXYBENZOIC ACID ANHYDRIDE - structure



AB Reaction of the pyrimidine I with (R1C6H4CO)2O (R1 = H, OH-o, -P, Me-o, -m, -p, NO2-o, Cl-o) gave the corresponding II and the oxazolopyrimidines III. III were methylated (MeI), acetylated, dehydrated, or cyclized with ClCO(CH2)nCOCl (n = 1, 2) to give IV-VII, resp.

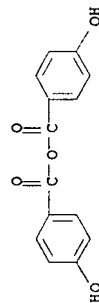
IT 61581-05-3

RL: RCT (Reactant); RACT (Reactant or reagent)

(reaction with diaminopyrimidinol)

61581-05-3 CAPLUS

CN Benzoic acid, 4-hydroxy-, anhydride (9CI) (CA INDEX NAME)



=> fil reg

COST IN U.S. DOLLARS

FULL ESTIMATED COST

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

CA SUBSCRIBER PRICE

SINCE FILE ENTRY 22.96

TOTAL SESSION 196.17

SINCE FILE ENTRY -3.12

TOTAL SESSION -3.12

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10/553451 CRY5 P-HYDROXYBENZOIC ACID ANHYDRIDE - structure

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STRUCTURE FILE UPDATES: 14 JUN 2007 HIGHEST RN 937362-79-3
DICTIONARY FILE UPDATES: 14 JUN 2007 HIGHEST RN 937362-79-3

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TSCA INFORMATION NOW CURRENT THROUGH December 2, 2006

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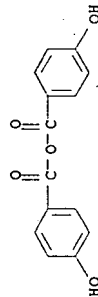
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predicted properties as well as tags indicating availability of
experimental property data in the original document. For information
on property searching in REGISTRY, refer to:

<http://www.cas.org/support/stngen/stdoc/properties.html>

=> s 61581-05-3/rn
L5 1 61581-05-3/RN

=> d l5

L5 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2007 ACS on STN
RN 61581-05-3 REGISTRY
ED Entered STN: 16 Nov 1984
CN Benzoic acid, 4-hydroxy-, anhydride (9CI) (CA INDEX NAME)
OTHER NAMES:
CN p-Hydroxybenzoic acid anhydride
MF C14 H10 O5
CI COM
LC STN Files: CA, CAPLUS, TOXCENTER



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

=> file caplu	SINCE FILE	TOTAL
COST IN U.S. DOLLARS	ENTRY	SESSION
FULL ESTIMATED COST	2.40	198.57
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	TOTAL

Page 9 searched 6/15/07

10/553451 CRY5 P-HYDROXYBENZOIC ACID ANHYDRIDE - structure

CA SUBSCRIBER PRICE ENTRY SESSION
0.00 -3.12

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FILE LAST UPDATED: 13 JUN 2007 (20070613/ED)

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=> d his

(FILE 'HOME' ENTERED AT 08:28:57 ON 15 JUN 2007)

FILE 'REGISTRY' ENTERED AT 08:29:10 ON 15 JUN 2007
L1 STRUCTURE UPLOADED
L2 0 S L1 SSS SAM
L3 3 S L1 SSS FULL

FILE 'CAPLUS' ENTERED AT 08:31:07 ON 15 JUN 2007
L4 4 S L3

FILE 'REGISTRY' ENTERED AT 08:33:14 ON 15 JUN 2007
L5 1 S 61581-05-3/RN

FILE 'CAPLUS' ENTERED AT 08:33:56 ON 15 JUN 2007
=> s l5 and "transition temperature"

1 L5
988581 "TRANSITION"
264538 "TRANSITIONS"
1102834 "TRANSITION"
(("TRANSITION" OR "TRANSITIONS")
628632 "TEMPERATURE"
81658 "TEMPERATURES"
697936 "TEMPERATURE"
(("TEMPERATURE" OR "TEMPERATURES")
3068948 "TEMP"
779803 "TEMES"
3408904 "TEMP"
(("TEMP" OR "TEMPS")
3568308 "TEMPERATURE"

Page 10 searched 6/15/07

10/553451 CRYs P-HYDROXYBENZOIC ACID ANHYDRIDE - structure

```
L6 140091 "TEMPERATURE" OR "TEMP"
    ("TRANSITION" (W) "TEMPERATURE")
    0 L5 AND "TRANSITION TEMPERATURE"

=> s "transition temperature"
    988581 "TRANSITION"
    264538 "TRANSITIONS"
    1102834 "TRANSITION"
    628632 "TEMPERATURE" OR "TRANSITIONS"
    81658 "TEMPERATURES"
    697936 "TEMPERATURE"
    3068948 "TEMP"
    779803 "TEMPS"
    3408904 "TEMP"
    ("TEMPERATURE" OR "TEMPERATURES")
    ("TEMP" OR "TEMPS")
    3568308 "TEMPERATURE"
    ("TEMPERATURE" OR "TEMP")
    140091 "TRANSITION TEMPERATURE"
    ("TRANSITION" (W) "TEMPERATURE")
```

```
=> s hydrate
    86394 HYDRATE
    28916 HYDRATES
    101545 HYDRATE
    (HYDRATE OR HYDRATES)
```

```
=> s l5 and l8
    1 L5
    0 L5 AND L8
```

```
=> s anhydride
    217738 ANHYDRIDE
    33390 ANHYDRIDES
    L10 228517 ANHYDRIDE
    (ANHYDRIDE OR ANHYDRIDES)
```

=> d his

```
(FILE 'HOME' ENTERED AT 08:28:57 ON 15 JUN 2007)
FILE 'REGISTRY' ENTERED AT 08:29:10 ON 15 JUN 2007
    STRUCTURE UPLOADED
    0 S L1 SSS SAM
    3 S L1 SSS FULL
FILE 'CAPLUS' ENTERED AT 08:31:07 ON 15 JUN 2007
    4 S L3
FILE 'REGISTRY' ENTERED AT 08:33:14 ON 15 JUN 2007
    1 S 61581-05-3/RN
FILE 'CAPLUS' ENTERED AT 08:33:56 ON 15 JUN 2007
    0 S L5 AND "TRANSITION TEMPERATURE"
    140091 S "TRANSITION TEMPERATURE"
    101545 S HYDRATE
    0 S L5 AND L8
```

Page 11 searched 6/15/07

10/553451 CRYs P-HYDROXYBENZOIC ACID ANHYDRIDE - structure

```
L10 228517 S ANHYDRIDE
=> s l8 and l10
    L11 2184 L8 AND L10
=> s l11 and l5
    1 L5
    L12 0 L11 AND L5
```

=> help operators
The following operators are available for use in searching: 'AND', 'OR', 'NOT', (W), (NOTW), (A), (NOTA), (P), (NOTP), (S), (NOTS), (L), (NOTL) and numeric operators. The order of precedence for the execution of operators is (highest first): numeric operators: (W), (NOTW), (A), and (NOTA); (S) and (NOTS); (P) and (NOTP); (L) and (NOTL); 'AND' and 'NOT'; then 'OR'. Parentheses (nesting) can be used to alter the order of execution. For example, the expression

=> SEARCH A AND B OR C NOT D

is equivalent to

=> SEARCH (A AND B) OR (C NOT D).

If the search logic required the set 'B OR C' to be combined with set A by 'AND' logic and set D by 'NOT' logic, parentheses would be required as shown below to produce the desired results.

=> SEARCH A AND (B OR C) NOT D

For more information on the individual operators, enter "HELP" and one of the following at an arrow prompt (=>): 'NUMERIC', '(NOTPROXIMITY)', 'AND', 'OR', 'NOT', (W), (A), (S), (P), or (L). Information on specific negative proximity operators is found with the corresponding positive proximity operator; e.g., for information on (NOTW), enter "HELP (W)". The numeric, Boolean, and (A), (NOTA), (W), and (NOTW) word proximity operators work the same in all files. However, the function of the (S), (NOTS), (P), (NOTP), (L), and (NOTL) operators depends on the data structure of the file you are in. Entering "HELP (S)", "HELP (P)", or "HELP (L)" will give information about how these operators work in the current file.

=> d his

```
(FILE 'HOME' ENTERED AT 08:28:57 ON 15 JUN 2007)
FILE 'REGISTRY' ENTERED AT 08:29:10 ON 15 JUN 2007
    STRUCTURE UPLOADED
    0 S L1 SSS SAM
    3 S L1 SSS FULL
FILE 'CAPLUS' ENTERED AT 08:31:07 ON 15 JUN 2007
    4 S L3
FILE 'REGISTRY' ENTERED AT 08:33:14 ON 15 JUN 2007
    1 S 61581-05-3/RN
FILE 'CAPLUS' ENTERED AT 08:33:56 ON 15 JUN 2007
    0 S L5 AND "TRANSITION TEMPERATURE"
```

Page 12 searched 6/15/07

10/553451 CRY5 P-HYDROXYBENZOIC ACID ANHYDRIDE - structure

L7 140091 S "TRANSITION TEMPERATURE"
L8 101545 S HYDRATE
L9 0 S L5 AND L8
L10 228517 S ANHYDRIDE
L11 2184 S L8 AND L10
L12 0 S L11 AND L5

=> s l5 and precipitation

1 L5
68195 PRECIPITATION
664 PRECIPITATIONS
68699 PRECIPITATION
(PRECIPITATION OR PRECIPITATIONS)

267038 PPTN
4375 PPTNS
269755 PPTN
(PPTN OR PPTNS)

291316 PRECIPITATION
(PRECIPITATION OR PPTN)
0 L5 AND PRECIPITATION

=> s l5 and precipitating

1 L5
4403 PRECIPITATING
38040 PPTG
41350 PRECIPITATING
(PRECIPITATING OR PPTG)
0 L5 AND PRECIPITATING

=> s l5/rgt

1 L5
46138 RGT/RL
0 L5/RGT
(L5 (L) RGT/RL)

=> s l5/proc

1 L5
4417183 PREP/RL
0 L5/PREP
(L5 (L) PREP/RL)

=> s l5/proc

1 L5
4118363 PROC/RL
0 L5/PROC
(L5 (L) PROC/RL)

=> s l5/pur

1 L5
257574 PUR/RL
0 L5/PUR
(L5 (L) PUR/RL)

=> s l5 and parahydroxybenzoic

1 L5
61 PARAHYDROXYBENZOIC
0 L5 AND PARAHYDROXYBENZOIC

=> fil casreact

10/553451 CRY5 P-HYDROXYBENZOIC ACID ANHYDRIDE - structure

COST IN U.S. DOLLARS SINCE FILE TOTAL
ENTRY 36.94 SESSION 235.51
FULL ESTIMATED COST
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) SINCE FILE TOTAL
ENTRY 0.00 SESSION -3.12
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FILE CONTENT:1840 - 9 Jun 2007 VOL 146 ISS 25

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This file contains CAS Registry Numbers for easy and accurate substance identification.

=> d his

(FILE 'HOME' ENTERED AT 08:28:57 ON 15 JUN 2007)

FILE 'REGISTRY' ENTERED AT 08:29:10 ON 15 JUN 2007

L1 STRUCTURE UPLOADED

L2 0 S L1 SSS SAM

L3 3 S L1 SSS FULL

FILE 'CAPLUS' ENTERED AT 08:31:07 ON 15 JUN 2007

L4 4 S L3

FILE 'REGISTRY' ENTERED AT 08:33:14 ON 15 JUN 2007

L5 1 S 61581-05-3/RN

FILE 'CAPLUS' ENTERED AT 08:33:56 ON 15 JUN 2007

L6 0 S L5 AND "TRANSITION TEMPERATURE"

L7 140091 S "TRANSITION TEMPERATURE"

L8 101545 S HYDRATE

L9 0 S L5 AND L8

L10 228517 S ANHYDRIDE

L11 2184 S L8 AND L10

L12 0 S L11 AND L5

L13 0 S L5 AND PRECIPITATION

L14 0 S L5 AND PRECIPITATING

10/553451 CRY5 P-HYDROXYBENZOIC ACID ANHYDRIDE - structure

L15 0 S L5/RGT
L16 0 S L5/PREP
L17 0 S L5/PROC
L18 0 S L5/PUR
L19 0 S L5 AND PARAHYDROXYBENZOIC

FILE 'CASREACT' ENTERED AT 08:47:29 ON 15 JUN 2007

=> s l5

L20 0 L5

=> e l5
E1 1 L42N8/BI
E2 1 L42NX2/BI
E3 166 --> L5/BI
E4 1 L50/BI
E5 1 L51784/BI
E6 27 L5178Y/BI
E7 1 L52/BI
E8 1 L5222/BI
E9 1 L52CU/BI
E10 1 L54M4/BI
E11 1 L55/BI
E12 1 L56/BI

=> s e3 or e6
166 "L5"/BI
27 L5178Y/BI

L21 193 "L5"/BI OR L5178Y/BI

=> d scan

L21 193 ANSWERS CASREACT COPYRIGHT 2007 ACS on STN

TI Extraction and coordination studies of the unexplored bifunctional ligand carbamoyl methyl sulfoxide (CMSO) with uranium(VI) and cerium(III) nitrates. Synthesis and structures of [UO2(NO3)2(PhSOCH2CONiBu2)] and [Ce(NO3)3(PhSOCH2CONBu2)2]
NO HIGHLIGHTING INFORMATION PRESENT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):5

L21 193 ANSWERS CASREACT COPYRIGHT 2007 ACS on STN

TI Synthesis, coordination to Rh(II), and hydroformylation catalysis of new β -aminophosphines bearing a dangling nitrogen group: an unusual inversion of a Rh-coordinated P center
NO HIGHLIGHTING INFORMATION PRESENT

L21 193 ANSWERS CASREACT COPYRIGHT 2007 ACS on STN

TI Sparsomycin analogs. V. Synthesis and antitumor activity of (E)- β -(pyrimidin-5-yl)acrylamides
NO HIGHLIGHTING INFORMATION PRESENT

L21 193 ANSWERS CASREACT COPYRIGHT 2007 ACS on STN

TI Betaine-induced assembly of neutral infinite columns and chains of linked silver(I) polyhedra with embedded acetylenediide

Page 15 searched 6/15/07

10/553451 CRY5 P-HYDROXYBENZOIC ACID ANHYDRIDE - structure

NO HIGHLIGHTING INFORMATION PRESENT

L21 193 ANSWERS CASREACT COPYRIGHT 2007 ACS on STN

TI Cobalt(II) and manganese(II) complexes of unsymmetric compartmental ligands bearing adjacent (N2O) and (N,S,O) donor sets
NO HIGHLIGHTING INFORMATION PRESENT

L21 193 ANSWERS CASREACT COPYRIGHT 2007 ACS on STN

TI Macrocyclic thioether-esters and thioether-thioesters and their palladium, platinum and silver complexes
NO HIGHLIGHTING INFORMATION PRESENT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):0

=> d l21 it

L21 ANSWER 1 OF 193 CASREACT COPYRIGHT 2007 ACS on STN

IT Michaelis constant
(kinetic parameters of protein kinases; preparation of nitrogen heterocyclic ruthenium metal complexes as glycogen synthase kinase 3 inhibitors)

IT Crystal structure

Molecular structure
(of pyridocarbazole cyclopentadienylruthenium complex)

IT Human
(preparation of nitrogen heterocyclic ruthenium metal complexes as glycogen synthase kinase 3 inhibitors)

IT 936112-70-8P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(crystal structure; preparation of nitrogen heterocyclic ruthenium metal complexes as glycogen synthase kinase 3 inhibitors)

IT 936112-68-4P

RL: PEP (Physical, engineering or chemical process); PRP (Properties); SPN (Synthetic preparation); PREP (Preparation); PROC (Process)
(mol. structure, HPLC chromatog. separation of isomers; preparation of nitrogen heterocyclic ruthenium metal complexes as glycogen synthase kinase 3 inhibitors)

IT 90698-26-3 114051-78-4, Lck kinase 137632-07-6, Erk1 kinase

141436-78-4, Protein kinase C α 144697-17-6, c-Src kinase

148047-34-1, ZAP-70 kinase 154907-65-0 391208-93-8, Glycogen synthase kinase 3 443900-93-6, Glycogen synthase kinase 3 β 53648-93-4,

Glycogen synthase kinase 3 α

RL: BCP (Biochemical process); BIOL (Biological study); PROC (Process)
(preparation of nitrogen heterocyclic ruthenium metal complexes as glycogen synthase kinase 3 inhibitors)

IT 936232-98-3P 936233-00-0P

RL: BSU (Biological study, unclassified); PAC (Pharmacological activity); PUR (Purification or recovery); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of nitrogen heterocyclic ruthenium metal complexes as glycogen synthase kinase 3 inhibitors)

IT 852658-41-4P 936112-65-1P 936112-66-2P 936112-69-5P

RL: BSU (Biological study, unclassified); PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

Page 16 searched 6/15/07

10/553451 CRY5 P-HYDROXYBENZOIC ACID ANHYDRIDE - structure

(preparation of nitrogen heterocyclic ruthenium metal complexes as glycoen
synthase kinase 3 inhibitors)
IT 3724-16-1, 3-Pyridineacetamide 80049-63-4 259752-98-2 936112-71-9
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of nitrogen heterocyclic ruthenium metal complexes as glycoen
synthase kinase 3 inhibitors)
IT 799822-53-0P 799822-54-1P 799822-55-2P 799822-56-3P 799822-57-4P
799822-58-5P 936112-67-3P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)
(preparation of nitrogen heterocyclic ruthenium metal complexes as glycoen
synthase kinase 3 inhibitors)

=> d his

(FILE 'HOME' ENTERED AT 08:28:57 ON 15 JUN 2007)

FILE 'REGISTRY' ENTERED AT 08:29:10 ON 15 JUN 2007

L1 STRUCTURE UPLOADED

L2 0 S L1 SSS SAM

L3 3 S L1 SSS FULL

FILE 'CAPLUS' ENTERED AT 08:31:07 ON 15 JUN 2007

L4 4 S L3

FILE 'REGISTRY' ENTERED AT 08:33:14 ON 15 JUN 2007

L5 1 S 61581-05-3/RN

FILE 'CAPLUS' ENTERED AT 08:33:56 ON 15 JUN 2007

L6 0 S L5 AND "TRANSITION TEMPERATURE"

L7 140091 S "TRANSITION TEMPERATURE"

L8 101545 S HYDRATE

L9 0 S L5 AND L8

L10 228517 S ANHYDRIDE

L11 2184 S L8 AND L10

L12 0 S L11 AND L5

L13 0 S L5 AND PRECIPITATION

L14 0 S L5 AND PRECIPITATING

L15 0 S L5/RGT

L16 0 S L5/PREP

L17 0 S L5/PROC

L18 0 S L5/PUR

L19 0 S L5 AND PARAHYDROXYBENZOIC

FILE 'CASREACT' ENTERED AT 08:47:29 ON 15 JUN 2007

L20 0 S L5

L21 E L5

193 S E3 OR E6

=> fil caplus

COST IN U.S. DOLLARS

SINCE FILE ENTRY

35.02

TOTAL SESSION

270.53

FULL ESTIMATED COST

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE ENTRY

0.00

TOTAL SESSION

-3.12

CA SUBSCRIBER PRICE

Page 17 searched 6/15/07

10/553451 CRY5 P-HYDROXYBENZOIC ACID ANHYDRIDE - structure

FILE 'CAPLUS' ENTERED AT 08:49:45 ON 15 JUN 2007
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FILE LAST UPDATED: 13 Jun 2007 (20070613/ED)

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They are available for your review at:

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=> s L21

L22 193 L21

=> s L22 and L7

L23 1 L22 AND L7

=> d ibib abs

L23 ANSWER 1 OF 1 CAPLUS. COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2005:1046581 CAPLUS

DOCUMENT NUMBER: 144:15951

TITLE: Lanthanide luminescent mesomorphic complexes with

macrocycles derived from diaza-18-crown-6

AUTHOR(S): Suarez, Stephane; Mamula, Olimpia; Scopelliti,

Rosario; Donnio, Bertrand; Guillon, Daniel; Terazzi,

Emmanuel; Piquet, Claude; Buenzli, Jean-Claude G.

LABORATORY OF Lanthanide Supramolecular Chemistry, BCH

1402, Ecole Polytechnique Federale de Lausanne (EPFL),

Lausanne, CH-1015, Switz.

SOURCE: New Journal of Chemistry (2005), 29(10), 1323-1334

CODEN: NJCHE5; ISSN: 1144-0546

PUBLISHER: Royal Society of Chemistry

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 144:15951

GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Four tetracatenar (L1-L4; I, Z = CH2, CO; R = OMe, OC10H21, OC12H25, OC18H33) and one hexacatenar (L5; I1) ligands, derived from the diaza-18-crown-6 framework, were synthesized and characterized. In these

Page 18 searched 6/15/07

ligands, the amine functions are fitted with benzoyloxybenzyl linker groups, attached either with a carbonyl function (L1) or a methylene bridge (L2-L5) and bearing alkoxy chains, R, of various lengths: R = OCH₃ for L2, OC10H₂₁ for L3 and L5, OC12H₂₅ for L1, and OC16H₃₃ for L4. The nonmesomorphic ligands L1 and L3-L5 react with various lanthanide salts to give complexes forming thermotropic hexagonal columnar phases, as ascertained by thermal, optical and small-angle x-ray diffraction methods. The length of the alkoxy chains (L3 and L4) does not much influence the mesogenic behavior, irrespectively of the linker function, the number of alkoxy chains, the counterion or the lanthanide ion. The best systems proved to be the nitrate lanthanide complexes with L3, which present a Colh phase over 100° (up to 147° for La) with melting transition temps. between 58 (La) and 86 (Tb) °C.

In the case of [Eu(NO₃)₃], chosen as a representative example of all the complexes in this anal., the inter-column separation of 29.2 Å agrees well with the packing of cylindrical columns resulting from an alternated side, i.e. stacking the mols. in a bent conformation. The liquid crystalline phases containing Eu and Tb display metal-centered emission, meaning that these complexes are interesting building blocks for the design of luminescent liquid crystalline materials.

REFERENCE COUNT: 57 THERE ARE 57 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> s l22 and precipitating
4403 PRECIPITATING
38044 PPTG
41354 PRECIPITATING
(PRECIPITATING OR PPTG)

L24 0 L22 AND PRECIPITATING

=> s l7 and l22
L25 1 L7 AND L22

=> d ibib abs

L25 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2005:1046581 CAPLUS
DOCUMENT NUMBER: 144:15951

TITLE: Lanthanide luminescent mesomorphic complexes with macrocycles derived from diaza-18-crown-6
AUTHOR(S): Suarez, Stephanie; Mamula, Olimpia; Scopelliti, Rosario; Donnio, Bertrand; Guillon, Daniel; Terazzi, Emmanuel; Piquet, Claude; Buenzli, Jean-Claude G. Laboratory of Lanthanide Supramolecular Chemistry, BCH 1402, Ecole Polytechnique Federale de Lausanne (EPFL), Lausanne, CH-1015, Switz.

CORPORATE SOURCE: New Journal of Chemistry (2005), 29(10), 1323-1334

SOURCE: CODEN: NJCHE5; ISSN: 1144-0546

PUBLISHER: Royal Society of Chemistry

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 144:15951

GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Four tetracatenar (L1-L4; I, Z = CH₂, CO; R = OMe, OC10H₂₁, OC12H₂₅, OC16H₃₃) and one hexacatenar (L5; I1) ligands, derived from the diaza-18-crown-6 framework, were synthesized and characterized. In these ligands, the amine functions are fitted with benzoyloxybenzyl linker groups, attached either with a carbonyl function (L1) or a methylene bridge (L2-L5) and bearing alkoxy chains, R, of various lengths: R = OCH₃ for L2, OC10H₂₁ for L3 and L5, OC12H₂₅ for L1, and OC16H₃₃ for L4. The nonmesomorphic ligands L1 and L3-L5 react with various lanthanide salts to give complexes forming thermotropic hexagonal columnar phases, as ascertained by thermal, optical and small-angle x-ray diffraction methods. The length of the alkoxy chains (L3 and L4) does not much influence the mesogenic behavior, irrespectively of the linker function, the number of alkoxy chains, the counterion or the lanthanide ion. The best systems proved to be the nitrate lanthanide complexes with L3, which present a Colh phase over 100° (up to 147° for La) with melting transition temps. between 58 (La) and 86 (Tb) °C.

In the case of [Eu(NO₃)₃], chosen as a representative example of all the complexes in this anal., the inter-column separation of 29.2 Å agrees well with the packing of cylindrical columns resulting from an alternated side, i.e. stacking the mols. in a bent conformation. The liquid crystalline phases containing Eu and Tb display metal-centered emission, meaning that these complexes are interesting building blocks for the design of luminescent liquid crystalline materials.

REFERENCE COUNT: 57 THERE ARE 57 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> fil stng
COST IN U.S. DOLLARS

FULL ESTIMATED COST

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

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FILE 'STNGUIDE' ENTERED AT 08:51:44 ON 15 JUN 2007
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LAST RELOADED: Jun 8, 2007 (20070608/UP).

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(FILE 'HOME' ENTERED AT 08:28:57 ON 15 JUN 2007)

FILE 'REGISTRY' ENTERED AT 08:29:10 ON 15 JUN 2007
STRUCTURE UPLOADED

L1 0 S L1 SSS SAM

L2 3 S L1 SSS FULL

FILE 'CAPLUS' ENTERED AT 08:31:07 ON 15 JUN 2007
L3 4 S L3

FILE 'REGISTRY' ENTERED AT 08:33:14 ON 15 JUN 2007

10/553451 Crys p-HYDROXYBENZOIC ACID ANHYDRIDE - structure

L5 1 S 61581-05-3/RN

FILE 'CAPLUS' ENTERED AT 08:33:56 ON 15 JUN 2007

L6 0 S L5 AND "TRANSITION TEMPERATURE"

L7 140091 S "TRANSITION TEMPERATURE"

L8 101345 S HYDRATE

L9 0 S L5 AND L8

L10 228517 S ANHYDRIDE

L11 2184 S L8 AND L10

L12 0 S L11 AND L5

L13 0 S L5 AND PRECIPITATION

L14 0 S L5 AND PRECIPITATING

L15 0 S L5/RGT

L16 0 S L5/PREP

L17 0 S L5/PROC

L18 0 S L5/PUR

L19 0 S L5 AND PARAHYDROXYBENZOIC

FILE 'CASREACT' ENTERED AT 08:47:29 ON 15 JUN 2007

L20 0 S L5

L21 E L5

193 S E3 OR E6

FILE 'CAPLUS' ENTERED AT 08:49:45 ON 15 JUN 2007

L22 193 S L21

L23 1 S L22 AND L7

L24 0 S L22 AND PRECIPITATING

L25 1 S L7 AND L22

FILE 'STNGUIDE' ENTERED AT 08:51:44 ON 15 JUN 2007

EAST Search History

6/18/07

Ref #	Hits	Search Query	DBs	Default Operator	Plurals	Time Stamp
L1	1	p-hydroxybenzoic adj acid adj anhydride	US-PGPUB; USPAT; USOCR; EPO; JPO; DERWENT	OR	ON	2007/06/15 09:29
L2	1	parahydroxybenzoic adj acid adj anhydride	US-PGPUB; USPAT; USOCR; EPO; JPO; DERWENT	OR	ON	2007/06/15 09:29
S4	49	"562/895".CCLS.	US-PGPUB; USPAT; USOCR	OR	ON	2007/06/12 20:25
S5	144	((RYUZO) near2 (UENO)).INV.	US-PGPUB; USPAT; USOCR	OR	ON	2007/01/03 11:31
S6	301	((RYUZO) near2 (UENO)).INV.	EPO; JPO; DERWENT	OR	ON	2007/01/03 11:31
S7	49	((MASAYA) near2 (KITAYAMA)).INV.	US-PGPUB; USPAT; USOCR	OR	ON	2007/01/03 11:33
S8	91	((MASAYA) near2 (KITAYAMA)).INV.	EPO; JPO; DERWENT	OR	ON	2007/01/03 11:33
S9	6	((NOBUTAKA) near2 (IZUMICHI)).INV.	US-PGPUB; USPAT; USOCR	OR	ON	2007/01/03 11:33
S10	6	((NOBUTAKA) near2 (IZUMICHI)).INV.	EPO; JPO; DERWENT	OR	ON	2007/01/03 11:33
S11	6	((MASAHARU) near2 (KITAKA)).INV.	US-PGPUB; USPAT; USOCR	OR	ON	2007/01/03 11:33
S12	7	((MASAHARU) near2 (KITAKA)).INV.	EPO; JPO; DERWENT	OR	ON	2007/01/03 11:34
S17	2	jp-2002316969-\$.did.	EPO; JPO; DERWENT	OR	ON	2007/01/05 08:24
S18	0	("2006/0264670").URPN.	USPAT	OR	ON	2007/01/05 08:34
S19	0	"crystalline hydroxybenzoic acid".clm.	US-PGPUB; USPAT; USOCR	OR	ON	2007/06/15 08:05
S20	1317	"hydroxybenzoic acid".clm.	US-PGPUB; USPAT; USOCR	OR	ON	2007/06/13 07:52

EAST Search History

S21	49	"562/895".CCLS.	US-PGPUB; USPAT; USOCR	OR	ON	2007/01/05 08:36
S22	0	S20 and S21	US-PGPUB; USPAT; USOCR	OR	ON	2007/01/05 08:36
S23	240	S20 and granul\$	US-PGPUB; USPAT; USOCR	OR	ON	2007/01/05 09:01
S24	188	S23 and @ad<="20030417"	US-PGPUB; USPAT; USOCR	OR	ON	2007/01/05 08:45
S25	34	S21 and process	US-PGPUB; USPAT; USOCR	OR	ON	2007/01/05 08:45
S26	2	("5606068").URPN.	USPAT	OR	ON	2007/01/05 08:44
S27	450	S20 and precipitat\$	US-PGPUB; USPAT; USOCR	OR	ON	2007/01/05 09:19
S28	357	S27 and @ad<="20030417"	US-PGPUB; USPAT; USOCR	OR	ON	2007/01/05 09:38
S29	68	S28 and granul\$	US-PGPUB; USPAT; USOCR	OR	ON	2007/01/05 08:58
S30	57	("5025036").URPN.	USPAT	OR	ON	2007/01/05 08:53
S31	0	("6120949").URPN.	USPAT	OR	ON	2007/01/05 08:56
S32	141	S28 and crystalline	US-PGPUB; USPAT; USOCR	OR	ON	2007/01/05 08:59
S33	0	"para-hydroxybenzoic acid or p-hydroxybenzoic acid or parahydroxybenzoic acid".clm.	US-PGPUB; USPAT; USOCR	OR	ON	2007/01/05 09:25
S34	77	"para-hydroxybenzoic acid".clm.	US-PGPUB; USPAT; USOCR	OR	ON	2007/06/13 09:51
S35	0	("4814498").URPN.	USPAT	OR	ON	2007/01/05 09:29
S36	1	("4827027").URPN.	USPAT	OR	ON	2007/01/05 09:32
S37	1	("5072036").URPN.	USPAT	OR	ON	2007/01/05 09:33
S38	1	("5532406").URPN.	USPAT	OR	ON	2007/01/05 09:33
S39	0	("6133475").URPN.	USPAT	OR	ON	2007/01/05 09:34
S40	2	("5124477").URPN.	USPAT	OR	ON	2007/01/05 09:35

EAST Search History

S41	230	"4-hydroxybenzoic acid".clm.	US-PGPUB; USPAT; USOCR	OR	ON	2007/01/05 10:05
S42	183	S41 and @ad<="20030417"	US-PGPUB; USPAT; USOCR	OR	ON	2007/01/05 09:38
S43	1	("6114157").URPN.	USPAT	OR	ON	2007/01/05 09:48
S44	62	"parahydroxybenzoic acid".clm.	US-PGPUB; USPAT; USOCR	OR	ON	2007/01/05 10:06
S45	0	("2003/0160205").URPN.	USPAT	OR	ON	2007/01/05 09:52
S46	0	("6673962").URPN.	USPAT	OR	ON	2007/01/05 09:53
S47	0	("6673962").URPN.	USPAT	OR	ON	2007/01/05 09:55
S48	6	"4-hydroxybenzoic acid".ti.	US-PGPUB; USPAT; USOCR	OR	ON	2007/01/05 10:05
S49	9	"parahydroxybenzoic acid".ti.	US-PGPUB; USPAT; USOCR	OR	ON	2007/01/05 10:06
S50	14	"para-hydroxybenzoic acid".ti.	US-PGPUB; USPAT; USOCR	OR	ON	2007/01/05 10:06
S51	52	"562/895".CCLS.	US-PGPUB; USPAT; USOCR; EPO	OR	ON	2007/06/12 20:25
S52	1363	"hydroxybenzoic acid".clm.	US-PGPUB; USPAT; USOCR; EPO; JPO	OR	ON	2007/06/13 07:52
S53	19107	hydroxybenzoic adj acid	US-PGPUB; USPAT; USOCR; EPO; JPO	OR	ON	2007/06/13 07:55
S54	103853	transition adj temperature	US-PGPUB; USPAT; USOCR; EPO; JPO	OR	ON	2007/06/13 07:53
S55	2154	S53 and S54	US-PGPUB; USPAT; USOCR; EPO; JPO	OR	ON	2007/06/13 07:53
S56	1164	S55 and crystalline	US-PGPUB; USPAT; USOCR; EPO; JPO	OR	ON	2007/06/13 07:54

EAST Search History

S57	809	S56 and @ad<="20030417"	US-PGPUB; USPAT; USOCR; EPO; JPO	OR	ON	2007/06/13 09:33
S58	6	hydroxybenzoic adj acid adj anhydride	US-PGPUB; USPAT; USOCR; EPO; JPO	OR	ON	2007/06/13 07:55
S59	19107	hydroxybenzoic adj acid	US-PGPUB; USPAT; USOCR; EPO; JPO	OR	ON	2007/06/13 09:33
S60	103853	transition adj temperature	US-PGPUB; USPAT; USOCR; EPO; JPO	OR	ON	2007/06/13 09:33
S61	2154	S59 and S60	US-PGPUB; USPAT; USOCR; EPO; JPO	OR	ON	2007/06/13 09:33
S62	1164	S61 and crystalline	US-PGPUB; USPAT; USOCR; EPO; JPO	OR	ON	2007/06/13 09:33
S63	809	S62 and @ad<="20030417"	US-PGPUB; USPAT; USOCR; EPO; JPO	OR	ON	2007/06/13 09:43
S64	466	S63 and anhydride	US-PGPUB; USPAT; USOCR; EPO; JPO	OR	ON	2007/06/13 09:34
S65	466	S64 and S61	US-PGPUB; USPAT; USOCR; EPO; JPO	OR	ON	2007/06/13 09:35
S66	50	"562/895".CCLS.	US-PGPUB; USPAT; USOCR	OR	ON	2007/06/13 09:42
S67	0	S65 and S66	US-PGPUB; USPAT; USOCR; EPO; JPO	OR	ON	2007/06/13 09:34
S68	0	S64 and S66	US-PGPUB; USPAT; USOCR; EPO; JPO	OR	ON	2007/06/13 09:35

EAST Search History

S69	0	"angle of repose"	US-PGPUB; USPAT; USOCR; EPO; JPO; DERWENT	OR	ON	2007/06/13 09:42
S70	8350	angle near3 repose	US-PGPUB; USPAT; USOCR; EPO; JPO; DERWENT	OR	ON	2007/06/13 09:42
S71	8291	angle near2 repose	US-PGPUB; USPAT; USOCR; EPO; JPO; DERWENT	OR	ON	2007/06/13 09:42
S72	3929	S71 and @ad<="20030417"	US-PGPUB; USPAT; USOCR; EPO; JPO	OR	ON	2007/06/13 09:51
S73	0	S63 and S72	US-PGPUB; USPAT; USOCR; EPO; JPO	OR	ON	2007/06/13 09:43
S74	19175	S59 or S60 and S72	US-PGPUB; USPAT; USOCR; EPO; JPO	OR	ON	2007/06/13 09:43
S75	1164	S74 and S62	US-PGPUB; USPAT; USOCR; EPO; JPO	OR	ON	2007/06/13 09:44
S76	709	S75 and anhydride	US-PGPUB; USPAT; USOCR; EPO; JPO	OR	ON	2007/06/13 09:44
S77	709	S76 and crystalline	US-PGPUB; USPAT; USOCR; EPO; JPO	OR	ON	2007/06/13 09:49
S78	6	hydroxybenzoic adj acid adj anhydride	US-PGPUB; USPAT; USOCR; EPO; JPO	OR	ON	2007/06/13 09:47
S79	1	S77 and S78	US-PGPUB; USPAT; USOCR; EPO; JPO	OR	ON	2007/06/13 09:47

EAST Search History

S80	159	S77 and precipitation	US-PGPUB; USPAT; USOCR; EPO; JPO	OR	ON	2007/06/13 09:49
S81	885	"para-hydroxybenzoic acid"	US-PGPUB; USPAT; USOCR; EPO; JPO	OR	ON	2007/06/13 09:51
S82	1000	"parahydroxybenzoic acid"	US-PGPUB; USPAT; USOCR; EPO; JPO	OR	ON	2007/06/13 09:51
S83	1206	(S81 or S82) and @ad<="20030417"	US-PGPUB; USPAT; USOCR; EPO; JPO	OR	ON	2007/06/13 09:52
S84	2	S83 and S72	US-PGPUB; USPAT; USOCR; EPO; JPO	OR	ON	2007/06/13 09:53
S85	43	S83 and S65	US-PGPUB; USPAT; USOCR; EPO; JPO	OR	ON	2007/06/13 09:54
S86	54	S83 and S63	US-PGPUB; USPAT; USOCR; EPO; JPO	OR	ON	2007/06/13 09:54
S87	1	"hydroxybenzoic acid anhydride". clm.	US-PGPUB; USPAT; USOCR	OR	ON	2007/06/15 08:06
S88	9	("4380587").URPN.	USPAT	OR	ON	2007/06/15 08:06
S89	125	hydroxybenzoic near3 anhydride	US-PGPUB; USPAT; USOCR; EPO; JPO; DERWENT	OR	ON	2007/06/15 08:06
S90	75	hydroxybenzoic near2 anhydride	US-PGPUB; USPAT; USOCR; EPO; JPO; DERWENT	OR	ON	2007/06/15 08:16
S91	5	"hydroxybenzoic anhydride"	US-PGPUB; USPAT; USOCR; EPO; JPO; DERWENT	OR	ON	2007/06/15 08:16

EAST Search History

S92	0	"parahydroxybenzoic anhydride"	US-PGPUB; USPAT; USOCR; EPO; JPO; DERWENT	OR	ON	2007/06/15 08:16
S93	0	"para-hydroxybenzoic anhydride"	US-PGPUB; USPAT; USOCR; EPO; JPO; DERWENT	OR	ON	2007/06/15 08:16
S94	5	hydroxybenzoic adj anhydride	US-PGPUB; USPAT; USOCR; EPO; JPO; DERWENT	OR	ON	2007/06/15 08:18
S95	5	p-hydroxybenzoic adj anhydride	US-PGPUB; USPAT; USOCR; EPO; JPO; DERWENT	OR	ON	2007/06/15 09:28